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# Photoionization cross section of InP:Fe

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The spectral dependence of the photoionization cross section of Fe doped in InP is determined by photocapacitance spectroscopy. The optical process of the carrier emission from the deep acceptor level of Fe is discussed from the results. For the crystal-field-split level of $Fe^{2+}$:$^5E$, the photoionization cross sections for the fundamental transitions of $^5E \rightarrow \Gamma_1$ and $\Gamma_{15} \rightarrow {}^5E$ are adequately described by the Lucovsky model. Those optical thresholds are 0.63 and 0.78 eV, respectively, at 77 K. In comparison with the deep-level transient spectroscopy measurements, the following conclusions are obtained. The energy separation between the Fe acceptor level and the conduction-band edge is constant, but that between the Fe level and the valence-band edge varies correspondingly to the temperature variation of the InP band-gap energy. The fact that there is no difference between the optical and thermal activation energies for the $^5E \rightarrow \Gamma_1$ transition indicates that the Fe acceptor level is not perturbed by the InP lattice vibration.

## I. INTRODUCTION

Fe is one of the major impurities that gives rise to the semi-insulating properties of InP. Since Fe is a midgap acceptor in InP, the transitions of electron emission to the conduction band and hole emission to the valence band, compete with each other.

Optical characterizations of InP:Fe have been performed using such techniques as deep-level optical spectroscopy (DLOS) of photoluminescence (PL),[1–4] photoconductivity (PC),[5,6] and photocapacitance (PHCAP).[1,7,8] Although accurate determinations of the optical thresholds for InP:Fe have been obtained from these experiments, a quantitative understanding of the capture and emission processes between the deep levels and their respective free-carrier bands is not presently available. The photoexcitation of carriers can be understood from the spectral dependence of the photoionization cross section which is obtained from the absolute value of the optical absorption coefficient of the deep-level impurity at a given atomic concentration. The optical absorption coefficient of the deep-level impurity is necessary to estimate the effects of the quantum efficiency in many optical devices.

We have performed a series of PHCAP measurements on InP:Fe from which the spectral dependence of the photoionization cross section has been determined. Optical thresholds have been obtained for the fundamental transitions by applying the Lucovsky model[9] to the analysis of the cross section. The effects of the InP lattice vibrations on the Fe acceptor have been analyzed by comparing the optical and thermal thresholds of Fe, while the energy separation between the Fe acceptor level and the band edges has also been studied as a function of temperature.

## II. EXPERIMENT

The Fe-doped InP crystal was grown by liquid-phase epitaxy (LPE) on (100)-oriented, Sn-doped, $n^+$-InP substrates at 850 °C. The InP growth melt was doped with 0.5 wt. % Fe and 0.1 wt. % Sn. The thickness of the InP epilayer was 5 $\mu$m. Cd was diffused into the wafer using $CdP_2$ as a diffusion source in a sealed ampoule at 550 °C for 60 min to form a $p^+$-$n$ abrupt junction in which the Cd-diffused region was 1.2 $\mu$m deep. AuZn was evaporated onto the $p^+$ side and alloyed for ohmic contacts while AuSn was used for the $n^+$-substrate side. Mesa-type $p^+$-$n$ junction diodes of 500 $\mu$m in diameter were fabricated by wet-chemical etching. The carrier concentration of the $n$-InP layer was determined from the 1-MHz capacitance-voltage measurements at room temperature to be $1 \times 10^{16}$ cm$^{-3}$, while the concentration of the Fe impurity was found to be $8.5 \times 10^{15}$ cm$^{-3}$.

PHCAP measurements were carried out by first cooling the diode from room temperature to 77 K in the dark at zero-bias voltage after which a 5-V reverse-bias voltage was applied, until a steady-state condition was obtained. The transient capacitance increase was recorded as a function of the time at 77 K after the diode was illuminated with excitation light to each of the wavelengths selected.

## III. RESULTS

The energy level scheme associated with the optical transitions under study is shown in Fig. 1 and consists of both the $^5E$ and $^5T_2$ crystal-field-split $Fe^{2+}$ ($3d^6$) levels, the conduction-band minima at CB($\Gamma_1$, $L_1$) and the valence-band minima at VB($\Gamma_{15}$). The energy separations of $\Delta E(\Gamma_1 - \Gamma_{15})$, $\Delta E(L_1 - \Gamma_1)$, and $\Delta E(^5T_2 - {}^5E)$ are 1.41, 0.5,[8] and 0.35 eV, respectively at 77 K.

Figure 2 is a logarithmic plot of the capacitance transient, in which $\Delta C(t)$ is the photocapacitance change at the

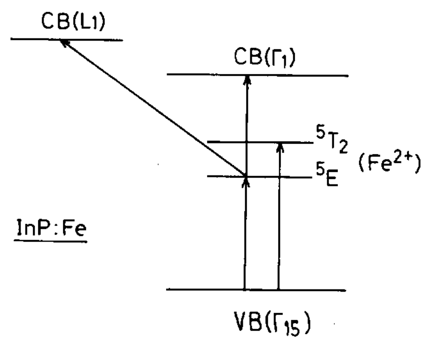


FIG. 1. Energy levels associated with the optical transitions in InP:Fe.

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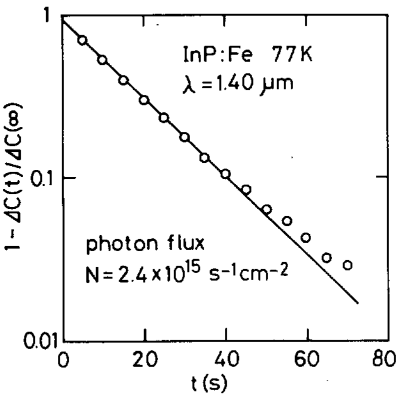


FIG. 2. Photocapacitance transient of the InP:Fe $p^+$-$n$ diode.

time $t$ and $\Delta C(\infty)$ is the full capacitance transient. The wavelength and the photon flux density of the incident light are $\lambda = 1.40\,\mu$m and $N = 2.4\times 10^{15}\ \mathrm{s}^{-1}\ \mathrm{cm}^{-3}$. The capacitance transient was also found to be exponential over the whole wavelength range studied.

Figure 3 is the plot of $\Delta C(\infty)$ as a function of the incident photon energy. The value of $\Delta C(\infty)$ is determined by the contributions from two competitive transitions involving electron emission to the conduction band and electron capture from the valence band, both of which share the same common Fe acceptor level.

The photoionization cross section of the Fe acceptor is determined from a suitable analysis of PHCAP measurement data. Carrier emission from the deep level to the respective carrier band is expressed by the equation

$$\frac{dn_t}{dt} = -\sigma_n^0 N n_t + \sigma_p^0 N p_t\,, \tag{1}$$

in which $n_t$ and $p_t$ are the trapped electron and hole densities, $N_t$ is the total trap concentration, and $N$ is the incident photon flux density, while $\sigma_n^0$ and $\sigma_p^0$ are the photoionization cross sections for electron and hole emission, respectively. In the steady state,

$$n_t(\infty) = N_t\,[\sigma_p^0/(\sigma_p^0 + \sigma_n^0)]\,, \tag{2}$$

while the full capacitance transient $\Delta C(\infty)$ is proportional to $N_t - n_t$. The emission rate $e^0$ is related to the photoionization cross sections by the equation

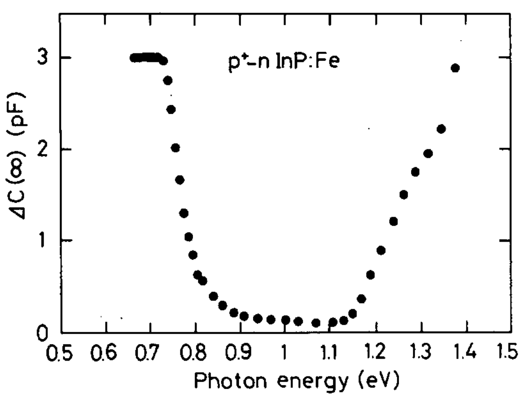


FIG. 3. Spectral dependence of the full capacitance transient.

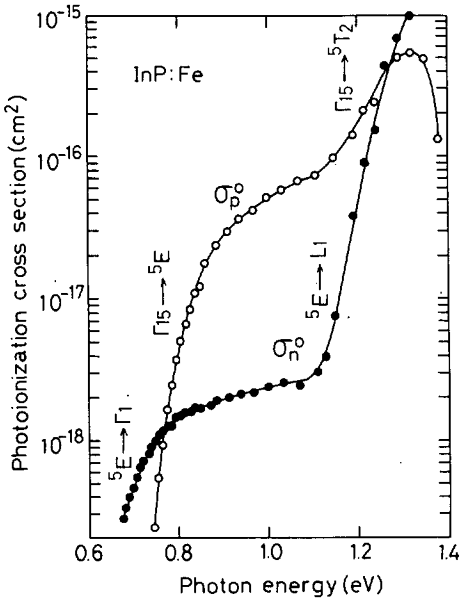


FIG. 4. Spectral dependence of the photoionization cross sections of InP:Fe.

$$e^0 = (\sigma_n^0 + \sigma_p^0)N\,. \tag{3}$$

$\sigma_n^0$ and $\sigma_p^0$ are determined by Eqs. (2) and (3).

The spectral dependence of the photoionization cross section of InP:Fe is shown in Fig. 4 which covers the range of measurements from 0.6 to 1.4 eV. Accurate measurements were not possible at $h\nu > 1.4$ eV because of the photocurrent generation from intraband absorption. The ${}^5E \rightarrow \Gamma_1$ electron is initiated at 0.63 eV. The indirect transition of ${}^5E \rightarrow L_1$ is added to the process at 1.13 eV, and $\sigma_n^0$ for this transition shows a strong dependence on the photon energy. The $\Gamma_{15} \rightarrow {}^5E$ electron capture is initiated at 0.78 eV and is followed by the $\Gamma_{15} \rightarrow {}^5T_2$ transition at 1.13 eV. Since $\sigma_p^0$ is larger than $\sigma_n^0$ in the range from 0.8 to 1.2 eV, electron capture from VB to the $Fe^{2+}$ level is expected to be dominant in this energy range. However, since $\sigma_n^0$ for the ${}^5E \rightarrow L_1$ transition is larger than $\sigma_p^0$ for $h\nu > 1.3$ eV, electron emission is the most important transition process near the InP band gap. Alter-

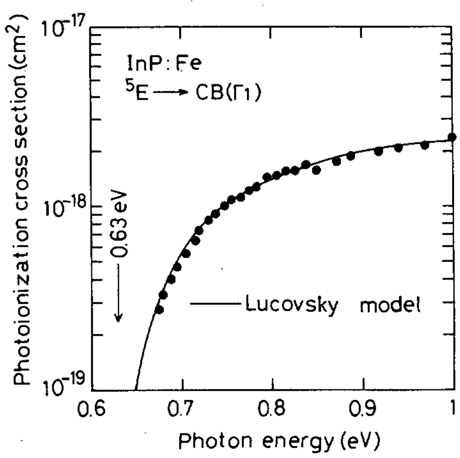


FIG. 5. Photoionization cross section for the ${}^5E \rightarrow \Gamma_1$ transition.



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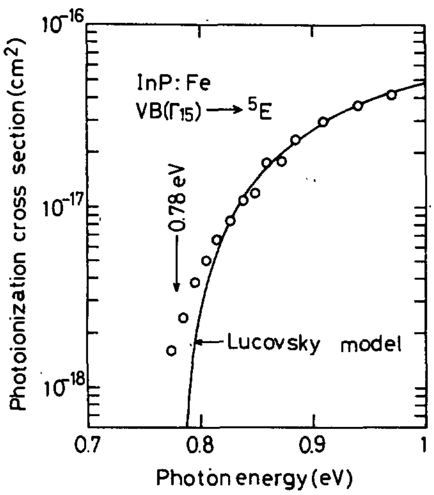


FIG. 6. Photoionization cross section for the $\Gamma_{15}\rightarrow{}^5E$ transition.

natively, $\sigma_p^0$ reaches a maximum value at 1.32 eV but decreases suddenly thereafter, which may be due to photocurrent generation.

The photoionization cross sections for the fundamental transitions ${}^5E\rightarrow\Gamma_1$ and $\Gamma_{15}\rightarrow{}^5E$ are described by the Lucovsky model[9]

$$\sigma_n^0({}^5E\rightarrow\Gamma_1) = 1.0\times10^{-17}[(h\nu-0.63)^{3/2}/(h\nu)^3]\ \text{cm}^2, \tag{4}$$

in which the optical threshold of 0.63 eV has been used. The calculated photoionization cross-section curve and the corresponding experimental data points are shown in Fig. 5 where good agreement between the two is seen.

The expression for the $\Gamma_{15}\rightarrow{}^5E$ transition is given by

$$\sigma_p^0(\Gamma_{15}\rightarrow{}^5E) = 4.8\times10^{-16}[(h\nu-0.78)^{3/2}/(h\nu)^3]\ \text{cm}^2, \tag{5}$$

where the optical threshold is 0.78 eV. The calculated and measured data are shown in Fig. 6, and from this we can conclude that the photoionization cross section of the deep level associated with the Fe acceptor in InP is adequately described by the Lucovsky model.

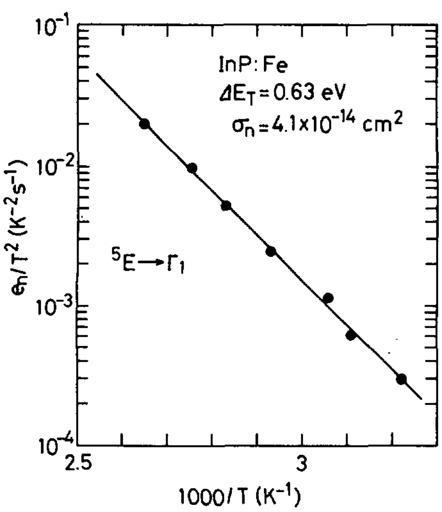


FIG. 7. Arrhenius plot for the Fe acceptor in InP.

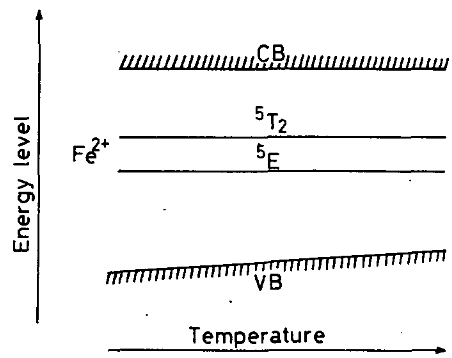


FIG. 8. Schematic temperature dependence of the energy levels in InP:Fe.

## IV. DISCUSSIONS

Let us first consider the difference between the optical and thermal energies for the Fe acceptor in InP. From the DLTS measurement, the thermal activation energy $\Delta E_T$ for the ${}^5E\rightarrow\Gamma_1$ transition is 0.63 eV, as determined from the Arrhenius plot in Fig. 7 which encompasses the temperature range from 330 to 380 K. And comparably, the same values of $\Delta E_T$ have been reported by others[1,7] for DLTS measurements on InP:Fe near room temperature. Since the relation

$$\Delta E_0(77\ \text{K})\geqslant\Delta E_T(77\ \text{K})\geqslant\Delta E_T(300\ \text{K}) \tag{6}$$

should be valid for the Fe deep level in InP, then $\Delta E_T$ for the ${}^5E\rightarrow\Gamma_1$ transition must be constant and equal to 0.63 eV from 77 to 300 K because $\Delta E_0$(77 K) and $\Delta E_T$(300 K) are each 0.63 eV. This result indicates that the energy separation between the ${}^5E$ level and the conduction band is constant, but that between the ${}^5E$ and the valence band, changes according to the temperature variation of the InP band gap are shown in Fig. 8. This conclusion is also valid for the ${}^5T_2$ level because the energy separation between the split ${}^5E$ and ${}^5T_2$ level is constant.

Since the Franck–Condon shift energy $d_{FC}$ ($=\Delta E_0 - \Delta E_T$) for the ${}^5E\rightarrow\Gamma_1$ transition is zero, it is concluded that the perturbation of the InP lattice vibration on the Fe acceptor level is very small. In the configuration-coordinate scheme, as shown in Fig. 9, the positions of the coordinates

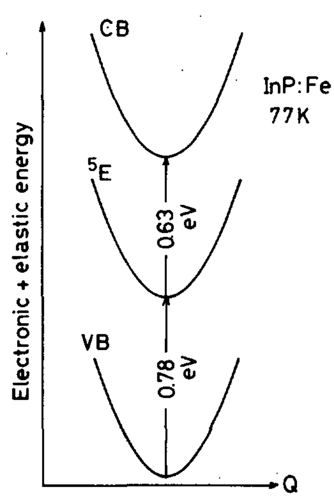


FIG. 9. Configuration-coordinate scheme for the energy levels of InP:Fe.



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at which the potential energies of each level have minima are coincident. The summation of the optical threshold energies for the $^5E \rightarrow \Gamma_1$ and $\Gamma_{15} \rightarrow {}^5E$ transitions determined in this study is equal to the InP band-gap energy at 77 K.

Fe-doped *n*-InP was studied in this experiment. However, there is a difference in concentrations of the possible charged states $Fe^{2+}$ and $Fe^{3+}$ between *n*-type and semi-insulating InP. The conditions are $[Fe^{2+}] \gg [Fe^{3+}]$ in *n*-InP and $[Fe^{3+}] \gg [Fe^{2+}]$ in semi-insulating InP. Klein, Furneaux, and Henry[10] have pointed out the differences in the mechanism and intensity of photoluminescence of the $^5T_2 \rightarrow {}^5E$ intra-atomic transition, which indicates the condition of the charged state. The strong transition initiated at 1.15 eV has been identified with electron emission from the $Fe^{3+}$ level to the conduction band by photoconductivity measurements on the semi-insulating InP:Fe at low temperatures.[6] The observed optical threshold is almost the same as that for the $^5E \rightarrow L_1$ transition in the present PHCAP measurement on the *n*-type InP:Fe.

## V. CONCLUSIONS

The photoionization cross section for the deep-level electronic transitions associated with the Fe acceptor in InP has been determined by photocapacitance spectroscopy. The photoionization cross-section formulations for the transitions of $^5E \rightarrow \Gamma_1$ and $\Gamma_{15} \rightarrow {}^5E$ have been determined. It is revealed that the energy separation between the Fe acceptor level and the conduction band is constant while that between the Fe level and the valence band is pinned to the temperature variation of the InP band gap. There is no difference between the observed optical and thermal thresholds in the $^5E \rightarrow \Gamma_1$ transition, which indicates the relatively weak phonon coupling between the Fe acceptor level and the InP crystal lattice.


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